

# Calculation of the two-body $T$ -matrix in configuration space.

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## Abstract

A spectral integral method (*IEM*) for solving the two-body Schrödinger equation in configuration space is generalized to the calculation of the corresponding  $T$ -matrix. It is found that the desirable features of the *IEM*, such as the economy of mesh-points for a given required accuracy, are carried over also to the solution of the  $T$ -matrix. However the algorithm is considerably more complex, because the  $T$ -matrix is a function of two variables  $r$  and  $r'$ , rather than only one variable  $r$ , and has a slope discontinuity at  $r = r'$ . For a simple exponential potential an accuracy of 7 significant figures is achieved, with the number  $N$  of Chebyshev support points in each partition equal to 17. For a potential with a large repulsive core, such as the potential between two *He* atoms, the accuracy decreases to 4 significant figures, but is restored to 7 if  $N$  is increased to 65.

## I. INTRODUCTION

The two-body  $T$ -matrix is most often used for the calculation of two-body scattering phase shifts by means of integrals, thereby avoiding the need to match the wave function to known asymptotic functions at large distances. For two-body scattering calculations a representation of the  $T$ -matrix in momentum space is most convenient because this space is most closely related to the ingoing and outgoing momenta of the scattering process. However, for other applications it is convenient to formulate the  $T$ -matrix, and its respective integral equation, in configuration space. One such application occurs for the solution in configuration space of the three-body Faddeev integral equations, which require as input the two-body scattering matrices for each of the three arrangements [1].

The function  $T(E; r, r')$  satisfies the integral equation

$$T(E; r, r') = V(r) \delta(r - r') + V(r) \int_0^\infty \mathcal{G}_0(E; r, \bar{r}) T(E; \bar{r}, r') d\bar{r} \quad (1)$$

Here  $\mathcal{G}_0$  is the undistorted (free) two-body Green's function  $\mathcal{G}_0 = (E + i\varepsilon - H_0)^{-1}$ , that, for a particular partial wave in configuration space with angular momentum  $\ell = 0$  is given by the well known expression

$$\mathcal{G}_0(E; r, \bar{r}) = -\frac{1}{k} F(E; r_<) G(E; r_>) \quad (2)$$

where  $F(E; r) = \sin(kr)$ ;  $G(E; r) = \cos(kr)$  or  $\exp(ikr)$ . In the case of  $\ell \neq 0$ ,  $F$  and  $G$  are replaced by the corresponding Bessel-Ricatti functions. Here  $k$  is the wave number in units of inverse length, and  $E$  and  $V(r)$  are the energy and the local two-body potential, in units of inverse length squared, respectively. In these units  $k = (E)^{1/2}$  (for negative energies  $\kappa = (-E)^{1/2}$ ).

The purpose of this paper is to present an algorithm for the solution of Eq. (1) for the two-variable function  $T(E; r, r')$  based on the use of spectral expansions in terms of Chebyshev polynomials [2], [3]. This method, denoted as *IEM*, has been found to be well suited for the solution of the one-variable Lippmann-Schwinger equation for the wave function  $\psi(r)$ , both for positive [4], [5] and negative [6] energies. One essential feature of the *IEM* is to divide the entire radial range into partitions, and expand the unknown function in each partition in terms of a small number ( $\simeq 17$ ) of basis functions such as Chebyshev or Legendre polynomials. Partitioning has the merit a) that the number of mesh points is

very economical, since the partitions are concentrated automatically in those regions where the function varies most rapidly, b) the accuracy control of the spectral expansions is also maintained, and c) the singularity in the driving term, described below, can be easily handled by placing the boundary between two partitions at the position of the singularity. The basic reason that partitioning can still be maintained for the calculation of  $T$  is that the integral in Eq. (1) is over one variable only, i.e., the second variable is introduced only parametrically through the driving term  $V(r) \delta(r - r')$ .

The properties of  $T$  in configuration space are little known, mainly because  $T$  has usually been studied in the momentum representation. However, the potential between atoms are generally given in configuration space, and the presence of large repulsive cores as well as long range parts of the potential, that become important at ultra-cold energies for atom-atom scattering, can cause difficulties in the momentum representation. It is hoped that a good understanding of  $T$  in configuration space can provide a simpler way for overcoming these difficulties. Another important motivation is that the solution of the three-body Faddeev integral equations in momentum space [7], [8] achieves an accuracy of three to four significant figures [9], which is adequate for nuclear physics applications, but is inadequate for atomic physics applications. In order to make use of the *IEM*'s high accuracy for the solution of integral equations in configuration space, the three-body Faddeev integral equations have been formulated in configuration space [1]. Since a basic input into these equations are integrals over the two-body  $T$ -matrices [10], knowledge of the properties of the two-body  $T$ -matrix in configuration space provides an important contribution.

## II. THE FORMALISM

An important relation between the  $T$ -matrix, the potential  $V$ , and the scattering wave function  $\psi$  is

$$V(r) \psi(r) = \int_0^\infty T(r, \bar{r}) F(\bar{r}) d\bar{r}. \quad (3)$$

Here  $\psi$  is the solution of the Schrödinger equation

$$-\frac{d^2\psi}{dr^2} + (V - k^2)\psi = 0 \quad (4)$$

or of the corresponding Lippmann- Schwinger (L-S) equation

$$\psi(r) = F(r) + \int_0^\infty \mathcal{G}_0(r, r') V(r') \psi(r') dr'. \quad (5)$$

Symbolically the solution of the L-S equation for  $\psi$  can be written as  $\psi = (1 - \mathcal{G}_0 V)^{-1} F$ , from which one finds  $T = V (1 - \mathcal{G}_0 V)^{-1}$ . The latter can be rewritten as  $T = (1 - V \mathcal{G}_0)^{-1} V$ , from which either Eq. (1) follows, or the alternate form

$$T(E; r, r') = V(r) \delta(r - r') + V(r') \int_0^\infty T(E; r, \bar{r}) \mathcal{G}_0(E; \bar{r}, r') d\bar{r}, \quad (6)$$

obtained by using the formal identity  $(1 - V \mathcal{G}_0)^{-1} V = V (1 - \mathcal{G}_0 V)^{-1}$ .

The function  $T(r, r')$  is symmetric in  $r$ , and  $r'$  as can be seen by comparing Eqs. (1) and (6) and making use of the symmetry of the Green's function  $\mathcal{G}_0$ . Even though the  $T$ -matrix has a discontinuous derivative at  $r = r'$ , as discussed below, the integral of the product of  $T$  with another function  $\Phi$

$$\bar{T}(E; r) = \int_0^\infty T(E, r, r') \Phi(r') dr' \quad (7)$$

over one of the two variables is a continuous function of the other variable, and obeys a continuous one-variable integral equation

$$\bar{T}(E; r) = V(r) \Phi(r) + V(r) \int_0^\infty \mathcal{G}_0(E; r, \bar{r}) \bar{T}(E; \bar{r}) d\bar{r}, \quad (8)$$

that can be solved without difficulty [10] using methods described earlier [2].

The first step in solving Eqs. (1) or (6) is to separate out the delta function term from  $T$  by defining  $R(r, r')$  according to

$$T(E; r, r') = V(r) \delta(r - r') + R(E; r, r'). \quad (9)$$

As a result of Eq. (1) the L-S equation for  $R$  becomes

$$R(E; r, r') = V(r) \int_0^\infty \mathcal{G}_0(E; r, \bar{r}) R(E; \bar{r}, r') d\bar{r} + V(r) \mathcal{G}_0(E; r, r') V(r'), \quad (10)$$

which is the object of the present numerical evaluation. One physical interpretation of  $R(E; r, r')$  is that its integral over  $F$  represents all second and higher order Born terms of the iterative solution of the L-S Eq. (5) for the wave function

$$\begin{aligned} \psi(r) = & F(r) + \int_0^\infty \mathcal{G}_0(E; r, \bar{r}) V(\bar{r}) F(\bar{r}) d\bar{r} \\ & + \int_0^\infty \mathcal{G}_0(E; r, \bar{r}) \left[ \int_0^\infty R(E; \bar{r}, r') F(r') dr' \right] d\bar{r}. \end{aligned} \quad (11)$$

This equation follows by inserting (1) into the right hand side of Eq. (3) and cancelling the potential  $V(r)$ . The second term involving  $R$  in Eq. (11) is likely to cancel the first two terms in the repulsive core region of  $V$  since  $\psi$  is small in this region, hence integrals over  $R$  alone are generally to be avoided.

### III. THE SPECTRAL METHOD

An extension of the conventional spectral expansion method *IEM* [2] for solving Eq. (10) is described in this section. For simplicity the energy variable is suppressed in what follows, and the driving term  $V(r)\mathcal{G}_0(E; r, r')V(r')$  is denoted as  $D(E; r, r')$ . In order to simplify the notation, it is useful to define the functions  $\mathfrak{F}$  and  $\mathfrak{G}$  as

$$\mathfrak{F}(E; r) = F(E; r)V(r) \quad (12)$$

$$\mathfrak{G}(E; r) = G(E; r)V(r) \quad (13)$$

in terms of which

$$D(E; r, r') = -\frac{1}{k}\mathfrak{F}(E; r_{<})\mathfrak{G}(E; r_{>}). \quad (14)$$

Since  $D$  has a discontinuous derivative at  $r = r'$ , the solution of Eq. (10) also acquires the same type of discontinuity.

Initially, without regard of the position of  $r'$ , the radial interval is truncated at an upper limit  $0 \leq r \leq r_{\max}$ , and that region is divided into  $M$  partitions. The size of each partition  $i$ , and the corresponding number  $M$  is determined automatically by the accuracy criterion according to the properties of Chebyshev expansions.[3], ([4]), and for this reason these partitions are denoted as Chebyshev partitions. The lower and upper limits of each partition are denoted by  $t_{i-1}$  and  $t_i$ , respectively,

$$t_{i-1} \leq r_i < t_i, \quad (15)$$

and if  $r$  is contained in partition  $i$  it is denoted as  $r_i$ . A second mesh of  $N_{rp}$  equidistant points  $r'$  is set up in the radial interval  $[0, r_{\max}]$  at a mesh distance of  $h_{rp}$ . For a point  $r'$  on this mesh that falls into a particular Chebyshev partition  $j$ , this partition is further divided into two, with  $r'$  located at the border between the two sub-partitions. The left (right) sub-partition is denoted as  $j_L$  ( $j_R$ ).

In what follows the energy is no longer written explicitly, and the angular momentum is assumed to be zero. The integral operator  $\mathcal{G}_0$  restricted to partition  $i$  is denoted as  $\mathcal{G}_i$  and is defined as

$$\mathcal{G}_i\xi \equiv -\frac{1}{k}G(r_i) \int_{t_{i-1}}^{t_i} F(\bar{r})\xi(\bar{r}) d\bar{r} - \frac{1}{k}F(r_i) \int_{r_i}^{t_i} G(\bar{r})\xi(\bar{r}) d\bar{r}, \quad (16)$$

where  $\xi$  is an arbitrary function being operated upon by  $\mathcal{G}_i$ . Inserting Eq. (9) into Eq.(10) one obtains

$$R_{i,j} - V(r_i)\mathcal{G}_i R_{i,j} = D(r_i, r'_j) + \mathfrak{G}(r_i) \int_0^{t_{i-1}} (-)\frac{1}{k}F(\bar{r}) R(\bar{r}, r'_j)d\bar{r} \\ + \mathfrak{F}(r_i) \int_{t_i}^{r_{\max}} (-)\frac{1}{k}G(\bar{r}) R(\bar{r}, r'_j)d\bar{r}. \quad (17)$$

where the left hand side of Eq. (17) denotes  $R(r_i, r'_j) - V(r_i) \int_{t_{i-1}}^{t_i} \mathcal{G}_0(r, \bar{r}) R(\bar{r}, r') d\bar{r}$ . The integrals in Eq.(17) do not depend on  $r$ , and are denoted as

$$A_i(r'_j) = -\frac{1}{k} \int_{t_i}^{r_{\max}} G(\bar{r}) R(\bar{r}, r'_j)d\bar{r} \quad (18)$$

$$B_i(r'_j) = -\frac{1}{k} \int_0^{t_{i-1}} F(\bar{r}) R(\bar{r}, r'_j)d\bar{r}. \quad (19)$$

In view of the linearity of the operator  $(1 - V\mathcal{G}_i)$  on the left hand side of Eq. 17, the solution of Eq. 17 can be written as [2] a linear combination of three functions  $Y$ ,  $Z$ , and  $S$

$$R(r_i, r'_j) = A_i(r'_j) Y_i(r_i) + B_i(r'_j) Z_i(r_i) + S_{i,j}(r_i, r'_j) \quad (20)$$

that are the solutions of

$$[1 - V(r_i)\mathcal{G}_i] Y_i = \mathfrak{F}(r_i) \quad (21)$$

$$[1 - V(r_i)\mathcal{G}_i] Z_i = \mathfrak{G}(r_i) \quad (22)$$

$$[1 - V(r_i)\mathcal{G}_i] S_{ij} = D(r_i, r'_j) \quad (23)$$

in each interval  $i$ . Up to here the procedure is identical to the *IEM* for the solution of two-body L-S equations. A new feature is the appearance of the third function  $S_{ij}$ , that, in view of Eq.(14) is given by

$$S_{ij}(r_i, r'_j) = -\frac{1}{k}Y_i(r_i) \mathfrak{G}(r'_j) \quad i < j \quad (24)$$

$$S_{ij}(r_i, r'_j) = -\frac{1}{k}Z_i(r_i) \mathfrak{F}(r'_j) \quad i > j. \quad (25)$$

For the partition  $j$  that subsequently was sub-divided into the left and right sub-partitions  $j_L$  and  $j_R$ , with  $r'_j$  at the border between the two partitions, Eqs. (24) and (25) remain valid for each of the sub-partitions, provided that  $i$  or  $j$  are replaced by the appropriate value  $j_L$  or  $j_R$ .

The calculations of the coefficients  $A$  and  $B$  is as follows. Inserting Eq.(20) into Eqs.(18) and (19) one obtains for  $i = 1, 2, ..M$

$$A_i(r'_j) = \sum_{h=i+1}^M v_h(r'_j) \quad (26)$$

$$B_i(r'_j) = \sum_{h=1}^{i-1} u_h(r'_j), \quad (27)$$

where

$$v_h(r'_j) = -A_h(r'_j) \langle GY \rangle_h - B_h(r'_j) \langle GZ \rangle_h - \langle GS \rangle_{h,j} \quad (28)$$

$$u_h(r'_j) = -A_h(r'_j) \langle FY \rangle_h - B_h(r'_j) \langle FZ \rangle_h - \langle FS \rangle_{h,j}. \quad (29)$$

In the above,

$$\langle \eta \xi \rangle_h = \int_{t_{h-1}}^{t_h} \frac{1}{k} \eta(\bar{r}) \xi_h(\bar{r}) d\bar{r}, \quad (30)$$

where  $\eta$  is either  $G$  or  $F$ , and  $\xi_h$  is either  $Y_h$  or  $Z_h$ , and

$$\langle \eta S \rangle_{h,j} = \int_{t_{h-1}}^{t_h} \frac{1}{k} \eta(\bar{r}) S_{h,j}(\bar{r}, r'_j) d\bar{r} \quad (31)$$

From Eqs. (26) and (27) it follows that  $B_1 = A_M = 0$ . In view of Eqs. (24) and (25) one obtains for the inhomogeneous overlap terms

$$\langle \eta S \rangle_{h,j} = -\frac{1}{k} \langle \eta Y \rangle_h \mathfrak{G}(x_j) \quad h < j \quad (32)$$

and

$$\langle \eta S \rangle_{h,j} = -\frac{1}{k} \langle \eta Z \rangle_h \mathfrak{F}(x_j) \quad h > j. \quad (33)$$

Here  $h$  stands for any of the partitions  $i = 1, 2, ..M$ , with the exception than when  $h = j$ ,  $h$  is replaced by either  $j_L$  or  $j_R$ . The equations above still apply, since  $r'_j$  is located either on the right or left border of the partition, respectively, as is explained in more detail below.

A recursion relation between the coefficients  $A_h$  and  $B_h$  and those from a neighboring partition  $h \pm 1$  can be obtained [4] by writing Eqs. (26) and (27) in the form

$$A_{h+1} - A_h = -v_{h+1} \quad (34)$$

$$B_{h+1} - B_h = u_h \quad (35)$$

According to Eqs. (28) and (29) the functions  $v_h$  and  $u_h$  contain the coefficients  $A_h$  and  $B_h$ , and hence, after some algebra one obtains, for  $i + 1$  and  $i$  both different from  $j$  [4]

$$\Omega_{i+1} \begin{pmatrix} A \\ B \end{pmatrix}_{i+1} = \Gamma_i \begin{pmatrix} A \\ B \end{pmatrix}_i + \begin{pmatrix} -\langle FS \rangle_{i,j} \\ \langle GS \rangle_{i+1,j} \end{pmatrix}; i = 1, 2, M - 1, \quad (36)$$

where

$$\Omega_{i+1} = \begin{pmatrix} 0 & 1 \\ 1 - \langle GY \rangle_{i+1} & -\langle GZ \rangle_{i+1} \end{pmatrix} \quad (37)$$

and

$$\Gamma_i = \begin{pmatrix} -\langle FY \rangle_i & 1 - \langle FZ \rangle_i \\ 1 & 0 \end{pmatrix}. \quad (38)$$

The matrices  $\Omega$  and  $\Gamma$  have already been defined in Ref. [4], while the terms in Eq. (36) involving the functions  $S$  are new

The method for obtaining the coefficients  $A_i$  and  $B_i$  as a function of  $r'_j$  consists in propagating the coefficients forward from partition  $i = 1$  to partition  $j_L$ , and backward, from partition  $M$  to  $j_L$ . By equating the two results in partition  $j_L$ , all the coefficients can be determined as a function of  $r'$ . These forward and backward propagations to the point  $r'_j$  bear some similarity to the method described in Ref. [6] for the calculation of energy eigenvalues of the Schrödinger equation. Further details for the calculation of the coefficients  $A_i$  and  $B_i$  are given in the Appendix 1. For  $i \neq j$  the result is a semi-separable expression of the form

$$R(r_i, r'_j) = [A_i(r'_j) - \mathfrak{G}(r'_j)/k] Y_i(r_i) + B_i(r'_j) Z_i(r_i), \quad i < j \quad (39)$$

$$R(r_i, r'_j) = A_i(r'_j) Y_i(r_i) + [B_i(r'_j) - \mathfrak{F}(r'_j)/k] Z_i(r_i), \quad i > j. \quad (40)$$

Integrals of  $R(r, r')$  over a known function  $\Phi(r)$ , as defined in Eq. (7), can be obtained by first calculating  $R$  and then performing the required integral, as is done below in order to check the accuracy of the results for  $R$ . However, a simpler and more accurate way is to solve the L-S equations (8) directly for these integrals. The present code can be modified for this purpose by replacing the driving term  $D$  in Eq. (14) by the continuous function  $V(r) \Phi(r)$  (no right or left sub-partitioning being required), calculating the function  $S$  in each partition according to Eq. (23), choosing an appropriate point  $r'$  at the boundary between two Chebyshev partitions, performing the forward and backward recursion relations for the quantities  $P, p$  and  $Q, q$ , respectively, and finally solving Eqs. (58) for the coefficients  $A_1$  and



$B_M$ . This operation has to be performed once only for the one point  $r'$  and can be carried out by the *IEM* with the same precision as the solution for the wave function [2], [4] or the binding energy [6].

If the driving term in Eq. (14) were set to zero, the quantities  $S_{i,j}$  in Eq. 23) would vanish, and hence Eq. (10) would be of the form

$$R(E; r, r') = V(r) \int_0^\infty \mathcal{G}_0(E; r, \bar{r}) R(E; \bar{r}, r') d\bar{r}. \quad (41)$$

The solution  $R$  of this equation vanishes, unless the determinant of the discretized form of the operator  $1 - V(r) \int_0^\infty d\bar{r} \mathcal{G}_0(E; r, \bar{r})$  is zero. This determinant does vanish for particular discrete energies which are the bound states of the two-body system. As the energy  $E$  ranges over the negative values which include bound state energies, poles in the  $R$ -matrix occur. However, the exploration of these singularities will be left to a future study.

### 1. Units and Dimensions

The potential energy  $\bar{V}$  and the energy  $\bar{E}$  in the Schrödinger equation are normally given in units of energy, while the distance is in units of length ( $\ell$ ). By multiplying all terms in the Schrödinger equation by  $2\mu/\hbar^2$ , where  $\mu$  is the reduced mass of the two colliding particles, and  $\hbar$  is Planck's constant divided by  $2\pi$ , then all terms in the scaled Schrödinger equation acquire dimensions of  $\ell^{-2}$ . The new potential energy  $V$  and the energy  $E$  then are

$$V = Q\bar{V} \quad (42)$$

$$E = k^2 = Q\bar{E} \quad (43)$$

where  $Q$  is a scaling factor.

For nuclear physics applications  $\bar{E}$  and  $\bar{V}$  are given in *MeV*, the radial distance in *fm* and the corresponding value of  $Q$  is

$$Q_N = 2\mu/\hbar^2. \quad (44)$$

The corresponding scaled Schrödinger equation is Eq. (4), and the corresponding L-S equation is (5). The dimension of the Green's function  $\mathcal{G}_0$ , Eq. (2), is  $\ell^1$  (for the nuclear case  $\ell \equiv fm$ ) and hence the operator  $\mathcal{G}_0(r, r')V(r')dr'$  has no dimension. In view of Eq. (3), and since  $F$  and  $\psi$  have no dimension, the  $T$ -Matrix has dimension  $\ell^{-3}$ . This dimension

is compatible with Eq. (9), since the delta function has dimension  $\ell^{-1}$ . The dimension of  $R$  is also  $\ell^{-3}$ , which is compatible with Eq. (10). The dimension of  $A$  and  $B$ , Eqs. (18) and (19), is  $\ell^{-1}$ , the dimension of  $Y$  and  $Z$ , Eqs. (21)-(22), is  $\ell^{-2}$ , and that of  $S$ , (23) is  $\ell^{-3}$ . The quantities  $\langle \eta \xi \rangle$ , Eq. (30), and  $\langle \eta S \rangle$  Eq. (31), have dimensions  $\ell^0$  and  $\ell^{-1}$ , respectively. The quantities  $\mathfrak{G}$  or  $\mathfrak{F}$  have dimensions  $\ell^{-2}$ , and hence Eqs. (39) and (40) are dimensionally self-consistent, each term having the dimension  $\ell^{-3}$ .

For atomic physics applications  $\bar{E}$  is given in atomic energy units  $2\mathbb{R}$ , ( $\mathbb{R} \simeq 13.606 \text{ eV}$ ) and the distance  $r$  in units of the Bohr radius  $a_0$ , in which case

$$Q_A = \frac{2\mu}{\hbar^2} a_0^2 \times 2\mathbb{R} = \frac{2\mu}{m_e}, \quad (45)$$

where  $m_e$  is the mass of the electron. In this case  $\bar{E}$  and  $r$ , and similarly the scaled quantities  $V$  and  $E$ , Eqs. (42) and (43), respectively, have no dimension and hence all the quantities described above for the nuclear case have no dimensions either.

#### IV. NUMERICAL EXAMPLES

Two different potentials in Eq. (4) are used for the numerical examples presented here. One is a simple exponential potential and the other is a potential describing the interaction between two Helium atoms, based on the potential  $TTY$  [11], [12]. For the He-He case a soft repulsive core is applied for a distance less than  $r_{cut} = 4.5$ . The numerical  $IEM$  calculations are carried out from  $r = 0$  to  $r = r_{max}$ , so as to include the effect of the core accurately. The value of the accuracy parameter is  $tol = 10^{-8}$ , and the wave number is  $k = 1.5$ . The potential and the wave number are in units of inverse length squared, and inverse length, respectively.

##### A. The exponential example.

The potential in Eq. (4) is  $V(r) = \pm \exp(-r)$ . The  $R$ -matrix for the repulsive case is shown in Fig (1), and the behavior of the diagonal part of  $R$  is shown in Fig. (2). The derivative discontinuity of  $R(r, r')$  at  $r = r'$  is clearly visible in Fig. (1), and it is also seen that  $R$  is large where the potential is large. These features are also present for the  $He - He$  case, described below.

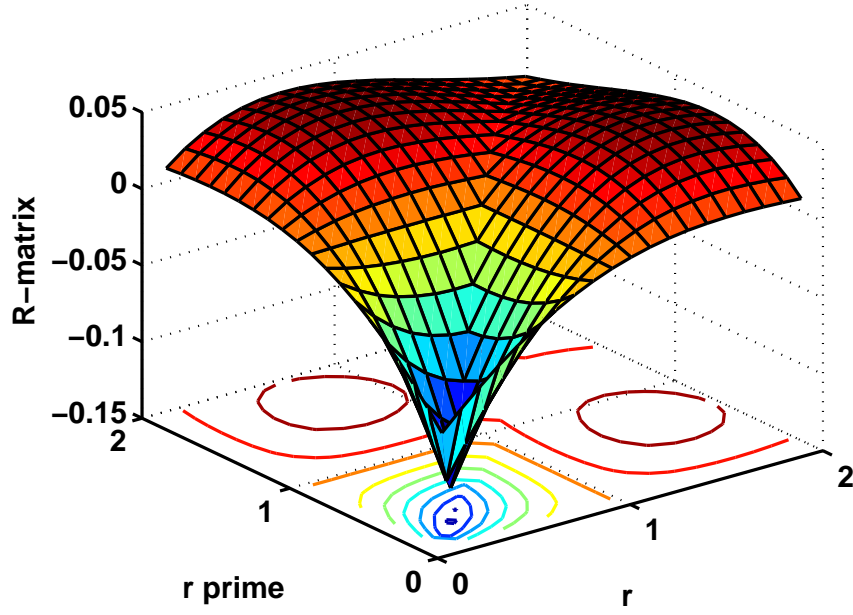


FIG. 1: The  $R$ -matrix for the exponential potential  $V = \exp(-r)$ . The wave number  $k$  is 1.5. The discontinuity in the derivative, for  $r = r'$  is clearly visible.

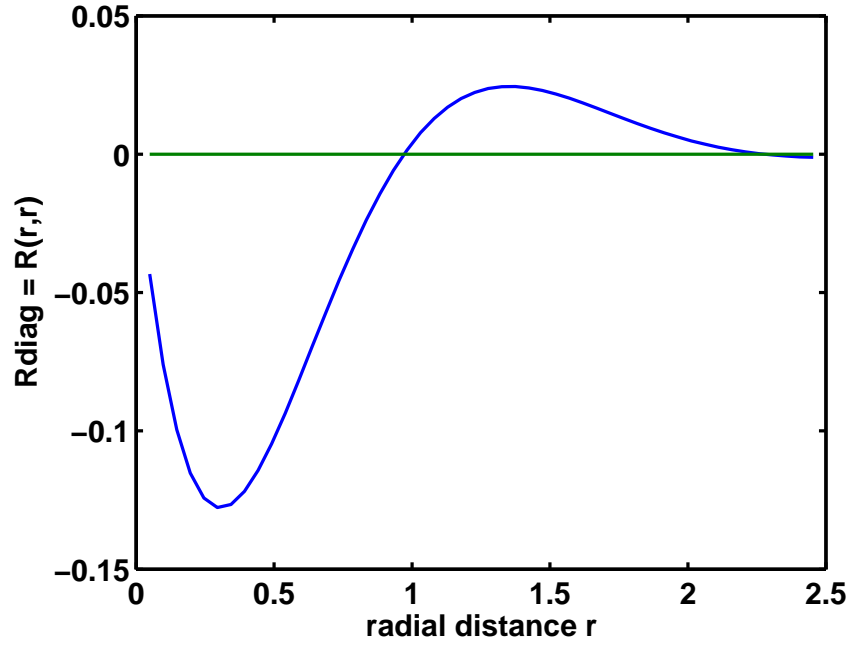


FIG. 2: The diagonal part of the  $R$ -matrix, shown in Fig. (1).

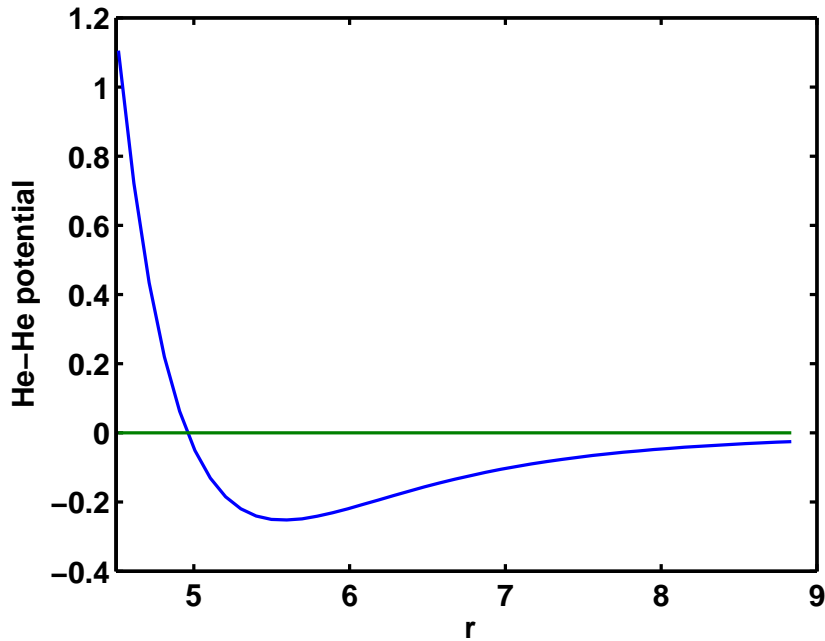


FIG. 3: The  $He - He$  atom interaction, based on the potential TTY [11]. The units for the distance are  $a_0$  (TheBohr radius) and  $(a_0)^{-2}$  for the potential. For distances less than  $4.5 a_0$  a repulsive soft core is matched to this potential, as described in the text. At  $r \simeq 0$  its value is  $\simeq 150 (a_0)^{-2}$ . The  $He - He$  dimer is very weakly bound, with a binding energy of  $2.58 \times 10^{-5} (a_0)^{-2}$ , or  $\simeq 10^{-7} eV$ . Upon division by the factor 7296.3 this potential is transformed to atomic energy units, as described in Ref.. [6].

### B. The He-He case.

For the  $He - He$  case the potential is shown in Fig. (3)

It has a strong repulsive core, that is not adequately represented by the formula described in Refs. [11],[12]. Since the result for the  $R$ -matrix depends significantly on the nature of the repulsive core, an "artificial" repulsive soft core was used to replace the repulsive core of  $TTY$  for distances  $0 < r \leq r_{cut}$ . This core is of the form  $a + br + cr^2$ , with the coefficients  $a, b$ , and  $c$  determined such that the repulsive core is equal to the value, the first, and second derivatives of  $TTY$  at  $r = r_{cut}$ . This form of the core is less unphysical than the "cut-off" core used in our previous numerical calculations of the binding energy of the  $He - He$  dimer [6], for which  $V$  was replaced by a constant value  $V(r_{cut})$  for  $0 < r \leq r_{cut}$ .

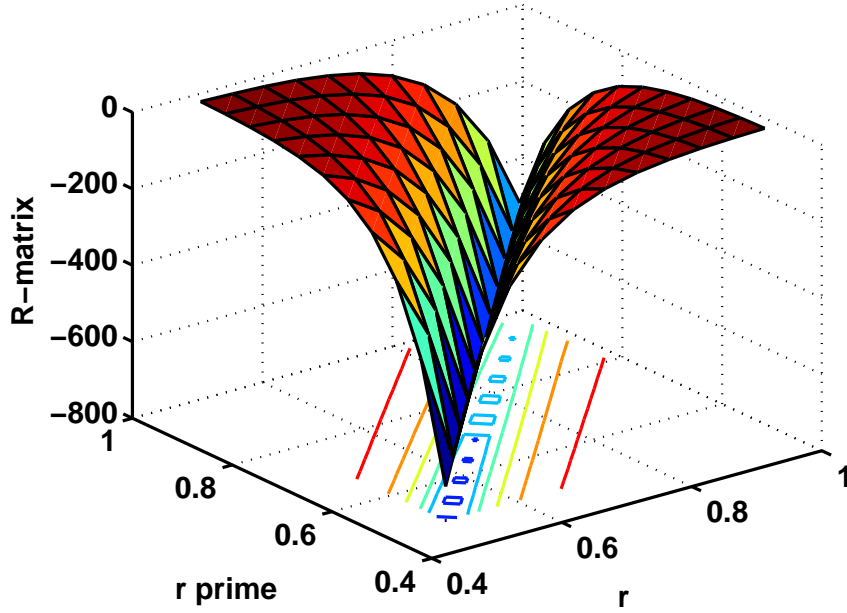


FIG. 4: The  $R$ -matrix for the  $He - He$  potential at distances well inside of the repulsive core, with  $r_{cut} = 4.5$ , and  $k = 1.5$ .

The  $R$ -matrix at small distances is shown in Fig. (4). The values of  $R$  are very large in the region of the large repulsive core, but they become smaller at larger distances, Figs. (5) and (6), for which the potential becomes progressively smaller.

The diagonal parts of the  $He - He$   $R$ -matrix are shown in Figs. (7) and (8), for short and large distances, respectively.

### C. Accuracy Tests.

The accuracy of the functions  $Y$  and  $Z$  in each partition, Eqs. (21) and (22), determined by the size of the partitions, is better than  $tol = 10^{-8}$ . In order to obtain a measure of the loss of accuracy that takes place in the subsequent steps of the calculation, the following two tests are performed: one that checks the symmetry of the  $R$ -matrix, and the other that performs the numerical integral

$$\mathfrak{I}(\mathfrak{r}') = \int_0^{r_{\max}} R(r, r') \times F(r) dr$$

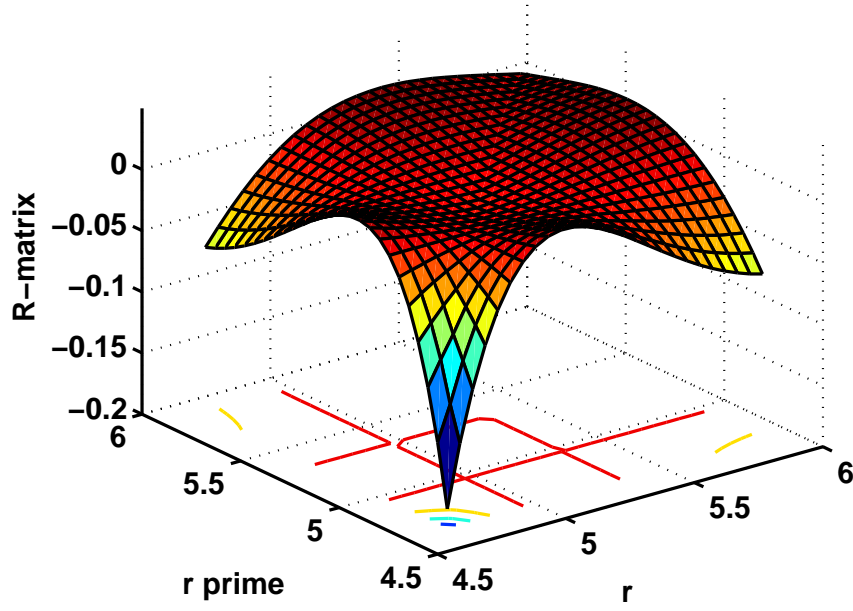


FIG. 5: The He-He  $R$ -matrix, same as in Fig. (4), but at larger distances, straddling the end of the repulsive core and the attractive potential valley.

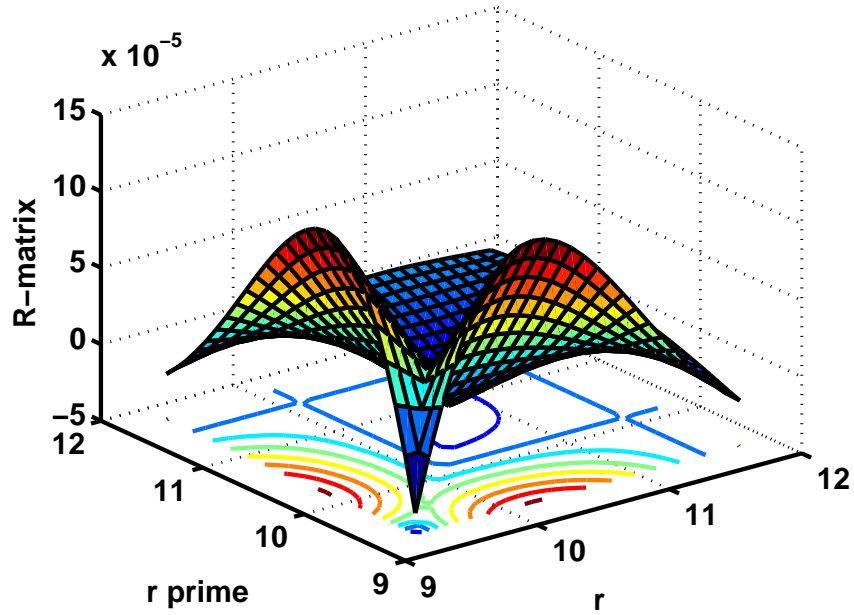


FIG. 6: The He-He  $R$ -matrix, same as in Fig. (4), at distances between 9 and 12  $a_0$  where the potential is of the  $r^{-6}$  form. The value of  $R$  is of the order of  $10^{-5} (a_0)^{-3}$ .

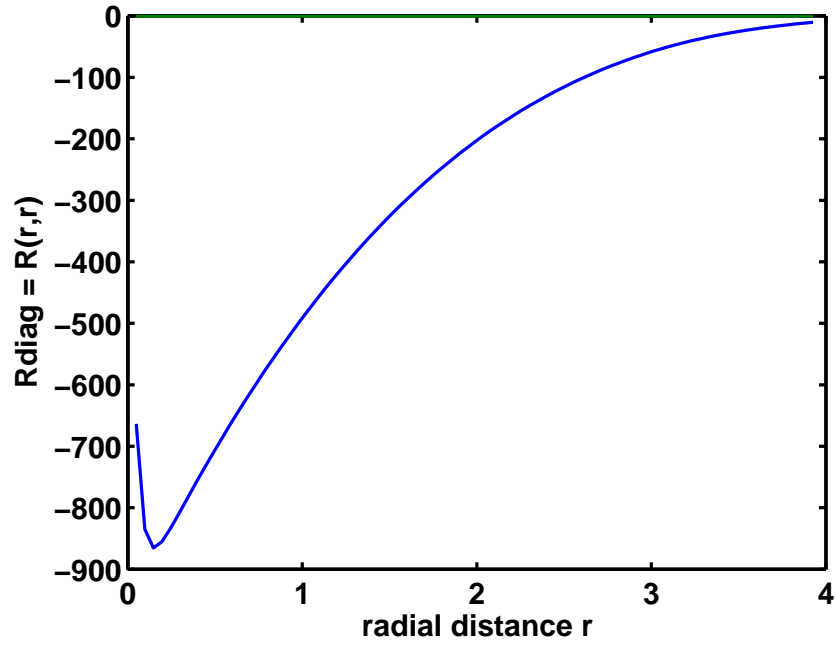


FIG. 7: The diagonal part of the  $He - He$   $R$ -matrix, shown in Fig. (4). at small distances

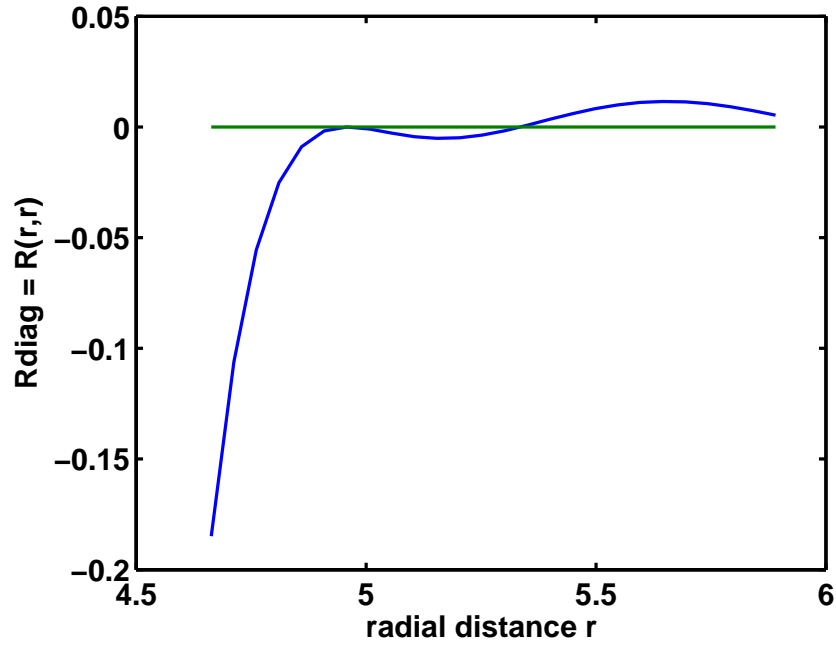


FIG. 8: Same as Fig. (7) for large distances.

$n$	$r = \frac{n \times \pi}{16}$		$Exp. \text{ pot'l}$	$He - He \text{ pot'l}$
10	$\simeq 1.96$	$L$	<b>3.85431605</b> [−2]	<b>−1.079593140</b> [1]
		$R$	3.85431605 [−2]	−1.079593140 [1]
15	$\simeq 2.95$	$L$	<b>4.05244938</b> [−3]	<b>2.34862829</b> [1]
		$R$	4.05244931 [−3]	2.34862833 [1]
20	$\simeq 3.93$	$L$	<b>−5.633010764</b> [−3]	<b>4.12156423</b>
		$R$	−5.633010723 [−3]	4.12156414
25	$\simeq 4.91$	$L$	<b>−1.073578042</b> [−3]	<b>1.4144533</b> [−2]
		$R$	−1.073578029 [−3]	1.4144530 [−2]
30	$\simeq 5.89$	$L$	<b>7.19293011</b> [−4]	<b>8.2459426</b> [−2]
		$R$	7.19293028 [−4]	8.2459429 [−2]
35	$\simeq 6.87$	$L$	<b>2.05522067</b> [−4]	<b>3.80032458</b> [−2]
		$R$	2.05522071 [−4]	3.80032395 [−2]
40	$\simeq 7.85$	$L$	<b>−8.59613654</b> [−5]	<b>1.9356054</b> [−2]
		$R$	−8.59613675 [−5]	1.9356055 [−2]

TABLE I: Values of the right (R) and left (L) sides of Eq. (46). Numbers in square brackets denote powers of 10

which, according to Eq. (3), should equal  $[\psi(r') - F(r')] V(r')$ .

$$\mathfrak{J}(r') = ? [\psi(r') - F(r')] V(r'), \quad (46)$$

In Table I the values of the two sides of the above equation are compared in order to check the accuracy of their agreement with each other. For the exponential case the number of Chebyshev support points in each partition is  $N = 17$ , and only four partitions are required to cover the interval from  $r = 0$  to  $r = 25$ .

For  $He - He$  case, if  $N = 17$ , the interval from 0 to 250 requires 26 partitions, 11 of which lie in the region of the repulsive core. The corresponding accuracy of the integral  $\mathfrak{J}(r)$  (not displayed in the table) is three to four significant figures. As  $N$  is increased, the size of each partition increases, correspondingly the number of partitions decreases. The accuracy of  $R$  increases the smaller the number of partitions, because the Chebyshev support points are the ones that carry the large change in the  $R$ -values, rather than the coefficients  $A$  and



*B.* The results for  $\mathfrak{J}(r)$  for  $N = 65$  are shown in "L" lines of Table (I), from which one can deduce an accuracy for  $R$  of at least 7 significant figures. For this case there are only four partitions in the region  $[0 \rightarrow 5]$  of the repulsive core, and four more partitions that cover the whole remaining distance  $[5 \rightarrow 250]$ . These accuracy results for both the exponential and the  $He - He$  cases are confirmed by the degree of symmetry of the  $R$ -matrix.

Using MATLAB, version 7.0.1.24704(R14) on a 2.8 GHz intel computer, the total time required for a  $He - He$  calculation of  $R(r, r')$ , with  $n = 1273$  equidistant meshpoints for each  $r$  and  $r'$ ,  $r_{\max} = 250$ ,  $N = 17$ , and  $tol = 10^{-8}$  requires 114 seconds. (This time scales like  $n^2$ ) For the same calculation, but with  $N = 65$ , the total MATLAB time is 261 s. The corresponding calculation of the wave function  $\psi$ , for  $r_{\max} = 1500$  and also 1273 equidistant meshpoints takes between 1 and 2 seconds.

## V. SUMMARY AND CONCLUSIONS

In this paper the spectral IEM method for solving the one variable Lippmann-Schwinger integral equation  $(L - S)$  in configuration space for the wave function [2],[4] is extended to the calculation of the two variable two-body  $T$ -matrix, also in configuration space. The  $T$ -matrix is written as the sum of a delta-function multiplying the (local) potential plus a reminder, called the  $R$ -matrix. The  $L - S$  equation for the latter is the object of the calculation. The main complication is that the driving term for this equation is continuous but has a discontinuous derivative at  $r = r'$ . That discontinuity also propagates into the  $R$ -matrix, and makes the calculation more cumbersome. This difficulty is overcome by constructing the partitions into which the radial domain is divided in such a way that the point  $r'$  is located at the end-point of a partition. This procedure is repeated for all values of  $r'$  contained in an equidistant set of mesh of points. Otherwise the calculation is very similar to the spectral *IEM* procedure for the solution of the one variable  $L - S$  equation, whose accuracy and reliability was previously demonstrated in various applications [5],[6]. The present method complements a previous investigation of expanding  $T$  in terms of a sum over Sturmian functions [13].

Two numerical examples are described. One, in which the potential is a simple exponential function of  $r$ , and the other in which the potential describes the interaction between two Helium atoms [11]. For the exponential case the high accuracy, which is determined by the

inputted tolerance parameter  $tol$ , is maintained. For  $tol = 10^{-8}$ , the  $R$ -matrix is accurate to 7 significant figures. For the  $He - He$  case the accuracy of  $R$  is reduced to between 3 and 4 significant figures. This loss of accuracy is attributed to the presence of the large repulsive core present in the  $He - He$  interaction. If the number of Chebyshev support points in each partition is increased from 17 to 65, then the accuracy of the  $R$ -matrix for the  $He - He$  case increases to 7 significant figures.

The calculation of integrals  $\bar{T}(r)$  over  $T(r, r')$  can be carried [10] out with far less computational effort than the calculation of  $T(r, r')$ , since these integrals can be obtained from the solution of a  $L - S$  equation (8) that is very similar to the  $L - S$  equation for the wave function, whose accuracy was found to be close to 7 or 8 significant figures [6]. This is of interest, since the integral Faddeev equations for the three-body system, formulated in configuration space [1] have such integrals as important inputs. It is our aim to investigate the numerical solution of the three-body integral Faddeev equations in configuration space in a future study, using the results of the present paper, and that of Ref. [10].

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## Appendix 1. The calculation of the coefficients A and B.

Implementing the solution of the recursion relations (36) in a numerically efficient way will be described below. A short summary is as follows. By implementing the forward recursion relations (47) described below, starting with  $(A_1, B_1) = (1, 0)$  one obtains the quantities  $P_i$  and  $p_i$ , Eq. 48), in terms of which the corresponding values of  $A_i$  and  $B_i$  for  $i < j$ , are given by  $(A_i, B_i)^T = A_1 P_i + p_i$ , Eq. (56) with  $A_1$  still unknown (here  $T$  means "transposed"). Similarly, the coefficients  $A_i$  and  $B_i$  are propagated backwards from the last partition  $M$  also into  $j_L$ , using Eq. (51), starting with  $(A_M, B_M) = (0, 1)$ , Eq. (56). The result is given by a combination of the quantities  $Q_i$  and  $q_i$ , Eq. 52). In terms of these quantities the corresponding coefficients  $A_i$  and  $B_i$  for and for  $i > j$  are given by

$(A_i, B_i)^T = B_M Q_i + q_i$ , Eq. (57) with  $B_M$  still unknown. By equating the coefficients  $A_{j_L}$  and  $B_{j_L}$  in the same partition  $j_L$ , obtained by the two procedures, one obtains two equations for the coefficients  $A_1$  and  $B_M$  in terms of the known "driving" terms  $p_i$  and  $q_i$  involving the functions  $S_{i,j}$ . These equations (58) then can be solved for  $A_1$  and  $B_M$ , but since they depend on the location of  $r'_j$ , the resulting values of  $A_1$  and  $B_M$  also depend on  $r'_j$ . By repeating this procedure for all values of  $r'_j$  in partition  $j$  for all partitions  $j$  one obtains  $A_i$  and  $B_i$  for all values of  $r'_j$ .

In detail the procedure is as follows. In view of Eq. (36) the "forward" recursion relations are

$$\begin{pmatrix} A^f \\ B^f \end{pmatrix}_{i+1} = (\Omega_{i+1})^{-1} \left\{ \Gamma_i \begin{pmatrix} A^f \\ B^f \end{pmatrix}_i + \frac{\mathfrak{G}(r'_j)}{k} \begin{pmatrix} \langle FY \rangle_i \\ -\langle GY \rangle_{i+1} \end{pmatrix} \right\}, \quad i = 1, 2, \dots, j-2. \quad (47)$$

In the above, when  $i = j-1$  then  $i+1 = j_L$ . By repeatedly using Eqs. (47) one can express  $A_i$  and  $B_i$  in terms of  $A_1$  and  $B_1$ , with the result

$$\begin{pmatrix} A^f \\ B^f \end{pmatrix}_i = P_i + p_i(j), \quad i = 2, 3, \dots, j-1, j_L, \quad (48)$$

where the recursion for the  $P_i$  and  $p_i$  column vectors for  $i = 1, 2, \dots, j-1$  are

$$P_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \quad P_{i+1} = \Omega_{i+1}^{-1} \Gamma_i P_i, \quad (49)$$

$$p_1 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}; \quad p_{i+1}(r'_j) = \Omega_{i+1}^{-1} \left[ \Gamma_i p_i(r'_j) + \frac{1}{k} \mathfrak{G}(r'_j) \begin{pmatrix} \langle FY \rangle_i \\ -\langle GY \rangle_{i+1} \end{pmatrix} \right]. \quad (50)$$

When  $i = j-1$ , the above expressions yield  $P_{j_L}$  and  $p_{j_L}$ .

The "backward" recurrence relations are

$$\begin{pmatrix} A^b \\ B^b \end{pmatrix}_{i-1} = (\Gamma_{i-1})^{-1} \left\{ \Omega_i \begin{pmatrix} A^b \\ B^b \end{pmatrix}_i + \frac{\mathfrak{F}(r'_j)}{k} \begin{pmatrix} -\langle FZ \rangle_{i-1} \\ \langle GZ \rangle_i \end{pmatrix} \right\}, \quad i = M, M-1, \dots, j+1. \quad (51)$$

When  $i = j+1$  then  $i-1$  is replaced by  $j_R$ . The superscripts  $f$  and  $b$  stand for "forward" and "backward", respectively. By repeatedly using Eq. (51) one obtains

$$\begin{pmatrix} A^b \\ B^b \end{pmatrix}_i = Q_i + q_i(j), \quad i = M-1, \dots, j+1, j_R \quad (52)$$

and the corresponding recursion relations for the  $Q_i$  and  $q_i$  column vectors are

$$Q_1 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}; \quad Q_{i-1} = \Gamma_{i-1}^{-1} \Omega_i Q_i \quad (53)$$

$$q_1 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}; \quad q_{i-1}(r'_j) = \Gamma_{i-1}^{-1} \left[ \Omega_i q_i(r'_j) + \frac{\mathfrak{F}(r'_j)}{k} \begin{pmatrix} -\langle FZ \rangle_{i-1} \\ \langle GZ \rangle_i \end{pmatrix} \right]. \quad (54)$$

In these expressions  $r'_j$  stands to the left of any partition, hence Eqs. (51) apply, and Eqs. (53) are valid for  $i - 1 = M - 2, M - 1, \dots, j_L$  while Eqs. (54) are valid only for  $i - 1 = M - 2, M - 1, \dots, j_R$ . For the backward recursion from  $j_R$  to  $j_L$  the expression for  $q_{j_L}$  has to be replaced by

$$q_{j_L}(r'_j) = \Gamma_{j_L}^{-1} \left[ \Omega_{j_R} q_{j_R}(r'_j) + \frac{1}{k} \begin{pmatrix} -\mathfrak{G}(r'_j) \langle FY \rangle_{j_L} \\ \mathfrak{F}(r'_j) \langle GZ \rangle_{j_R} \end{pmatrix} \right] \quad (55)$$

The vectors  $P_i$  for  $i < j$  and  $Q_i$  for  $i > j$  are independent of  $r'_j$  and the corresponding vectors  $p_i$  and  $q_i$  all dependent on  $r'_j$  via the factor  $\mathfrak{G}(r'_j)/k$  and  $\mathfrak{F}(r'_j)/k$  respectively, a feature that provides economy in the numerical calculation. The vectors  $(A^f, B^f)^T$  as given by Eq. (48) are the values of the coefficients  $A$  and  $B$  when the values of  $(A_1, B_1)^T$  in the first partition are set to  $(1, 0)^T$  and similarly for  $(A^b, B^b)^T$ , as given by Eq. (52), when the values of  $(A_M, B_M)^T$  in the last partition  $M$  are set to  $(0, 1)^T$ . The correct values of  $(A, B)^T$  are obtained by multiplying the vectors  $P_i$  by  $A_1$  and the vectors  $Q_i$  by  $B_M$ , i.e.,

$$\begin{pmatrix} A \\ B \end{pmatrix}_i = A_1(r'_j) P_i + p_i(r'_j), \quad i = 2, 3, \dots, j - 1, j_L, \quad (56)$$

$$\begin{pmatrix} A \\ B \end{pmatrix}_i = B_M(r'_j) Q_i + q_i(r'_j), \quad i = M - 1, \dots, j + 1, j_R. \quad (57)$$

In order to determine the values of  $A_1$  and  $B_M$  one equates to each other the values of  $(A, B)^T$  obtained by Eqs. (56) and (57), respectively, in the partition  $j_L$  with the result

$$\begin{pmatrix} P^{(1)} - Q^{(1)} \\ P^{(2)} - Q^{(2)} \end{pmatrix}_{j_L} \begin{pmatrix} A_1 \\ B_M \end{pmatrix} = q_{j_L} - p_{j_L}. \quad (58)$$

The procedure described above is repeated for every value of  $r'$  in partition  $j$ . A convenient set of such values, denoted as  $r'_{j,s'}$ ,  $s' = 1, 2, \dots, N + 1$ , which originate from in the equidistant mesh of points  $r'$  and are located in the Chebyshev mesh  $j$ .

The case when  $i = j$  is as follows, but for clarity of notation the subscript  $j$ , is suppressed. Each  $L_{s'}$  and  $R_{s'}$  partition has its own  $N + 1$  Chebyshev support points by means of which the Chebyshev expansion coefficients of the functions  $Y_{L_{s'}}$  and  $Z_{L_{s'}}$ , as well as  $Y_{R_{s'}}$  and  $Z_{R_{s'}}$  are calculated via the *IEM* in the Left and Right sub-partitions. By means of these expansion coefficients the values of the functions  $Y$  and  $Z$ , and hence also the values of these functions at a point  $r$  contained in the equidistant set of mesh-points can be calculated, and hence the functions  $R$  can be obtained at the equidistant mesh points of  $r$  and  $r'$ . In a simplified notation,  $R_j(s, s') = [A(s') - \mathfrak{G}(s')/k] Y_{L_{s'}}(s) + B(s') Z_{L_{s'}}(s)$ ,  $s \leq s'$ , and a similar expression based on Eq. (40) for  $s > s'$ .

After the cases that the points  $r$  are contained in different Chebyshev partitions than point  $r'$ , are combined with the case where  $r$  and  $r'$  are contained in the same Chebyshev partition, one obtains the final result for  $R(r_s, r'_{s'})$ . The dimension of this matrix is equal to the number  $N_{rp}$  of equidistant mesh points.

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